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# $\mathcal{PT}$ -symmetry and its spontaneous breakdown explained by anti-linearity

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## Abstract

The impact of an anti-unitary symmetry on the spectrum of non-hermitean operators is studied. Wigner's normal form of an anti-unitary operator is shown to account for the spectral properties of non-hermitean,  $\mathcal{PT}$ -symmetric Hamiltonians. Both the occurrence of single real or complex conjugate pairs of eigenvalues follows from this theory. The corresponding energy eigenstates span either one- or two-dimensional irreducible representations of the symmetry  $\mathcal{PT}$ . In this framework, the concept of a spontaneously broken  $\mathcal{PT}$ -symmetry is not needed.

Deep in their hearts, many quantum physicists will renounce hermiticity of operators only reluctantly. However, non-hermitean Hamiltonians are applied successfully in nuclear physics, biology and condensed matter, often modelling the interaction of a quantum system with its environment in a phenomenological way. Since 1998, non-hermitean Hamiltonians continue to attract interest from a conceptual point of view [1]: surprisingly, the eigenvalues of a one-dimensional harmonic oscillator Hamiltonian remain *real* when the *complex* potential  $\hat{V} = i\hat{x}^3$  is added to it. Numerical, semiclassical, and analytic evidence [2] has been accumulated confirming that bound states with *real* eigenvalues exist for the vast class of *complex* potentials satisfying  $V^\dagger(\hat{x}) = V(-\hat{x})$ . In addition, pairs of complex conjugate eigenvalues occur systematically.

$\mathcal{PT}$ -symmetry has been put forward to explain the observed energy spectra. The Hamiltonian operators  $\hat{H}$  under scrutiny are invariant under the combined action of parity  $\mathcal{P}$  and time reversal  $\mathcal{T}$ ,

$$[\hat{H}, \mathcal{PT}] = 0. \quad (1)$$

They act on the fundamental observables according to

$$\mathcal{P} : \begin{cases} \hat{x} \rightarrow -\hat{x}, \\ \hat{p} \rightarrow -\hat{p}, \end{cases} \quad \mathcal{T} : \begin{cases} \hat{x} \rightarrow \hat{x}, \\ \hat{p} \rightarrow -\hat{p}, \end{cases} \quad (2)$$

and  $\mathcal{T}$  *anti-commutes* with the imaginary unit,

$$\mathcal{T}i = i^*\mathcal{T} \equiv -i\mathcal{T}. \quad (3)$$

Whenever a  $\mathcal{PT}$ -symmetric Hamiltonian has a *real* eigenvalue  $E$ , the associated eigenstate  $|E\rangle$  is found to be an eigenstate of the symmetry  $\mathcal{PT}$ ,

$$E = E^* : \quad \hat{H}|E\rangle = E|E\rangle, \quad \mathcal{PT}|E\rangle = +|E\rangle. \quad (4)$$

Occasionally,  $\mathcal{PT}|E\rangle = -|E\rangle$  occurs [3] which is equivalent to (4) upon redefining the phase of the state:  $\mathcal{PT}(i|E\rangle) = +(i|E\rangle)$ . There is no difference between symmetry and anti-symmetry under  $\mathcal{PT}$ .

However, if the eigenvalue  $E$  is *complex*, the operator  $\mathcal{PT}$  does *not* map the corresponding eigenstate of  $\hat{H}$  to itself,

$$E \neq E^* : \quad \hat{H}|E\rangle = E|E\rangle, \quad \mathcal{PT}|E\rangle \neq \lambda|E\rangle, \text{ any } \lambda. \quad (5)$$

This situation is described as a ‘spontaneous breakdown’ of  $\mathcal{PT}$ -symmetry. No mechanism has been identified which would explain this breaking of the symmetry.

The  $\mathcal{PT}$ -symmetric square-well model provides a simple example for this behavior [4]. It describes a particle moving between reflecting boundaries at  $x = \pm 1$ , in the presence of a piecewise constant complex potential,

$$V_Z(x) = \begin{cases} iZ, & x < 0, \\ -iZ, & x > 0, \end{cases} \quad Z \in \mathbb{R}. \quad (6)$$

Acceptable solutions of Schrödinger’s equation must satisfy both the boundary conditions,  $\psi(\pm 1) = 0$ , and continuity conditions at the origin. As long as the value of the parameter  $Z$  is below a critical value,  $Z < Z_0^c$ , the eigenvalues  $E_n$  of the non-hermitean Hamiltonian  $\hat{H} = -\partial_{xx} + V_Z(x)$  are real, and each eigenstate  $|\psi_n\rangle$  satisfies the relations (4), with eigenvalues  $E_n$  and  $+1$ , respectively. Above the threshold,  $Z > Z_0^c$ , at least one pair of complex conjugate eigenvalues  $E_0$  and  $E_0^*$  develops. One of the corresponding eigenstates has the form [4]

$$\psi_0(x) = \begin{cases} K_p \sinh \kappa(1-x), & x > 0, \\ K_n \sinh \lambda^*(1+x), & x < 0, \end{cases} \quad (7)$$

the complex parameters  $\kappa, \lambda, K_n$ , and  $K_p$  being determined by the boundary and continuity conditions. The state  $\psi_0(x)$  is not invariant under  $\mathcal{PT}$ , i.e. (5) holds.

The purpose of the present contribution is a group-theoretical analysis of  $\mathcal{PT}$ -symmetry. The properties of  $\mathcal{PT}$ -symmetric systems are explained in a natural way by taking into account that  $\mathcal{PT}$  is not a unitary but an *anti-unitary* symmetry of a *non-hermitean* operator. The argument proceeds in three steps. First, Wigner’s normal form of anti-unitary operators is reviewed, i.e. their (irreducible) representations are identified. Second, the properties of non-hermitean operators with anti-unitary symmetry are derived. These results are then shown to account for the characteristic features of  $\mathcal{PT}$ -symmetric systems.

Wigner develops a normal form of anti-unitary operators  $\hat{A}$  in [5]. Anti-unitarity of  $\hat{A}$  is defined by the relation

$$\langle \hat{A}\chi | \hat{A}\psi \rangle = \langle \psi | \chi \rangle \quad (8)$$

and it implies anti-linearity,

$$\hat{A}(\alpha|\psi\rangle + \beta|\chi\rangle) = \alpha^*\hat{A}|\psi\rangle + \beta^*\hat{A}|\chi\rangle. \quad (9)$$

which is equivalent to (3). The representation theory of  $\hat{A}$  relies on the fact that the square of an anti-unitary operator is *unitary*:

$$\langle \hat{A}^2\chi | \hat{A}^2\psi \rangle = \langle \hat{A}\psi | \hat{A}\chi \rangle = \langle \chi | \psi \rangle. \quad (10)$$

Therefore, the operator  $\hat{A}^2$  has a complete, orthonormal set of eigenvectors  $|\Omega\rangle$  with eigenvalues  $\Omega$  of modulus one,

$$\hat{A}^2|\Omega\rangle = \Omega|\Omega\rangle, \quad |\Omega| = 1. \quad (11)$$

It plays the role of a Casimir-type operator labelling different representations of  $\hat{A}$ . Wigner distinguishes three different types of representations corresponding to the eigenvalues of  $\hat{A}^2$ : complex  $\Omega$  ( $\neq \Omega$ ),  $\Omega = +1$ , or  $\Omega = -1$ , summarized in Table (1).

1. An eigenstate  $|\Omega\rangle$  of  $\hat{A}^2$  with eigenvalue  $\Omega$  ( $\neq \Omega^*$ ) is not invariant under  $\hat{A}$ . Instead, the states  $|\Omega\rangle$  and  $|\Omega^*\rangle \equiv \hat{A}|\Omega\rangle$  constitute a ‘flipping pair’ with complex ‘flipping value’  $\omega$  (and  $\omega^*$ ), where  $\omega^2 = \Omega$ . They span a two-dimensional space which is closed under the action of  $\hat{A}$ . Therefore, it carries a two-dimensional representation of  $\hat{A}$ , denoted by  $\Gamma_*$ , which is *irreducible*: due to the anti-linearity of  $\hat{A}$ , no (non-zero) linear combination of the flipping states exist which is invariant under  $\hat{A}$ .
2. Similarly, if  $\hat{A}^2$  has an eigenvalue  $\Omega = -1$ , then the operator  $\hat{A}$  flips the states  $|-\rangle$  and  $|-*\rangle \equiv \hat{A}|-\rangle$ . The flipping value is  $i$ , and the associated two-dimensional representation  $\Gamma_-$  is not reducible.
3. Two different situations arise if there is an eigenstate  $|1\rangle$  of  $\hat{A}^2$  with eigenvalue  $+1$ . The state  $\hat{A}|1\rangle$  is either a multiple of itself or not. In the first case, the space spanned by  $|1\rangle$  is invariant under  $\hat{A}$  and hence carries a one-dimensional representation  $\gamma_+$  of  $\hat{A}$ . When redefining the phase of the state appropriately, one obtains an eigenstate  $|1\rangle$  of  $\hat{A}$  with eigenvalue  $+1$ . In the second case, the two states  $|+\rangle \equiv |1\rangle$  and  $|+^*\rangle \equiv \hat{A}|1\rangle$  provide a flipping pair with flipping value  $\omega = +1$ , and hence a representation  $\Gamma_+$ . This representation, however, is *reducible* due to the reality of the flipping value: the linear combinations  $|1_r\rangle = |+\rangle + |+^*\rangle$  and  $|1_i\rangle = i(|+\rangle - |+^*\rangle)$  are both eigenstates of  $\hat{A}$  with eigenvalue  $+1$ .

$\Omega \equiv \omega^2$	$\Gamma$	action of $\hat{A}$	$\dim \Gamma$
$\Omega \neq \Omega^*$	$\Gamma_*$	$\hat{A} \Omega\rangle = \omega^* \Omega^*\rangle$ $\hat{A} \Omega^*\rangle = \omega \Omega\rangle$	2
-1	$\Gamma_-$	$\hat{A} -\rangle = -i -*\rangle$ $\hat{A} -*\rangle = +i -\rangle$	2
+1	$\Gamma_+$	$\hat{A} +\rangle = + +^*\rangle$ $\hat{A} +^*\rangle = + +\rangle$	2
+1	$\gamma_+$	$\hat{A} 1\rangle = + 1\rangle$	1

Table 1: Representations  $\Gamma$  of the operator  $\hat{A}$

Consequently, a Hilbert space  $\mathcal{H}$  naturally decomposes into a direct product of invariant subspaces, each invariant under the action of the anti-unitary operator  $\hat{A}$ ,

$$\mathcal{H} = \Gamma_*^{\otimes N_*} \otimes \Gamma_-^{\otimes N_-} \otimes \Gamma_+^{\otimes N_+} \otimes \gamma_+^{\otimes n_+}; \quad (12)$$

the nonnegative integers  $N_*$ ,  $N_{\pm}$  and  $n_+$  are related to the degeneracies of the eigenvalues  $\Omega (\neq \Omega^*)$  and  $\Omega = \pm 1$  of the operator  $\hat{A}^2$ . The corresponding decomposition of a vector  $|\psi\rangle \in \mathcal{H}$  is the closest analog of an expansion into the eigenstates of a hermitean (or unitary) operator. Surprisingly, *two*-dimensional irreducible representations of  $\hat{A}$  exist although there is only one generator,  $\hat{A}$ . No ‘good quantum number’ exists which would label the states spanning these representations.

A (diagonalizable) *non-hermitean* Hamiltonian  $\hat{H}$  with a discrete spectrum [6] and its adjoint  $\hat{H}^\dagger$  each have a complete set of eigenstates:

$$\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle, \quad \hat{H}^\dagger|\psi^n\rangle = E^n|\psi^n\rangle, \quad (13)$$

with complex conjugate eigenvalues related by  $E^n = E_n^*$ . They form a *bi-orthonormal* basis in  $\mathcal{H}$ , as they provide two resolutions of unity,

$$\sum_n |\psi^n\rangle\langle\psi_n| = \sum_n |\psi_n\rangle\langle\psi^n| = \hat{I}, \quad (14)$$

and satisfy orthogonality relations,

$$\langle\psi_m|\psi^n\rangle = \delta_m^n. \quad (15)$$

Let the non-hermitean operator  $\hat{H}$  have an anti-unitary symmetry  $\hat{A}$ ,

$$[\hat{H}, \hat{A}] = 0. \quad (16)$$

Then the unitary operator  $\hat{A}^2$  commutes with  $\hat{H}$ , and it has eigenvalues  $\Omega$  of modulus one. Consequently, there are simultaneous eigenstates  $|n, \Omega\rangle$  of  $\hat{H}$  and  $\hat{A}^2$ :

$$\hat{H}|n, \Omega\rangle = E_n|n, \Omega\rangle, \quad \hat{A}^2|n, \Omega\rangle = \Omega|n, \Omega\rangle, \quad E_n \in \mathbb{C}. \quad (17)$$

For simplicity, the eigenvalues  $\Omega$  are assumed discrete and not degenerate. Wigner's normal form of anti-unitary operators suggests to consider three cases separately: complex  $\Omega$  ( $\neq \Omega^*$ ) and  $\Omega = \pm 1$ .

$\Omega \neq \Omega^*$  The state

$$|n, \Omega^*\rangle \equiv \omega \hat{A}|n, \Omega\rangle, \quad \omega^2 = \Omega, \quad (18)$$

is a second eigenstate of  $\hat{A}^2$ , with eigenvalue  $\Omega^*$ . The states  $\{|n, \Omega\rangle, |n, \Omega^*\rangle\}$  provide a *flipping pair* under the action of the operator  $\hat{A}$ ,

$$\hat{A}|n, \Omega\rangle = \omega^*|n, \Omega^*\rangle, \quad \hat{A}|n, \Omega^*\rangle = \omega|n, \Omega\rangle, \quad (19)$$

carrying the representation  $\Gamma_*$ . No degeneracy of the eigenvalue  $E_n$  is implied by the anti-unitary  $\hat{A}$ -symmetry of  $\hat{H}$ . However, the non-hermitean Hamiltonian has a second eigenstate  $|n, \Omega^*\rangle$  with eigenvalue  $E_n^*$ ,

$$\hat{H}|n, \Omega^*\rangle = E_n^*|n, \Omega^*\rangle, \quad (20)$$

as follows from multiplying the first equation of (17) with  $\hat{A}$  and  $\omega$ .

$\Omega = -1$  Formally, the results for the representation  $\Gamma_-$  are obtained from the previous case by setting  $\omega = i$ . Again, a pair of complex conjugate eigenvalues is found, and the associated flipping pair spans a two-dimensional representation space.

$\Omega = +1$  This case is conceptually different from the previous ones as two possibilities arise. Consider the state  $|n, +\rangle$ , an eigenvector of both  $\hat{H}$  and  $\hat{A}^2$  with eigenvalues  $E_n$  and  $+1$ , respectively. It satisfies Eqs. (17) with  $\Omega \rightarrow +$ . If, on the one hand, applying  $\hat{A}$  to  $|n, +\rangle$  results in  $e^{i\phi}|n, +\rangle$ , then the state  $|n, 1\rangle \equiv e^{-i\phi/2}|n, +\rangle$  is an eigenstate of  $\hat{A}$  with eigenvalue  $+1$ ,

$$\hat{A}|n, 1\rangle = |n, 1\rangle. \quad (21)$$

This occurrence of the one-dimensional representation  $\gamma_+$  forces the associated eigenvalue  $E_n$  of  $\hat{H}$  to be real since

$$E_n|n, 1\rangle = \hat{H}\hat{A}|n, 1\rangle = \hat{A}\hat{H}|n, 1\rangle = E_n^*|n, 1\rangle. \quad (22)$$

If, on the other hand,  $|n, +^*\rangle \equiv \hat{A}|n, +\rangle$  is *not* a multiple of  $|n, +\rangle$ , then these states combine to form the representation  $\Gamma_+$ , the flipping value being  $+1$ . Further, the state  $|n, +^*\rangle$  is an eigenstate of the Hamiltonian with eigenvalue  $E_n^*$ . As the flipping number is real, linear combinations of  $|n, +\rangle$  and  $|n, +^*\rangle$  do exist which are eigenstates of  $\hat{A}$ —however, they are not eigenstates of  $\hat{H}$ . Consequently, the anti-unitary symmetry of the Hamiltonian makes itself felt (on a subspace with  $(\mathcal{PT})^2 = +\hat{I}$ ) by either a single real eigenvalue or a pair of two complex conjugate eigenvalues.

If any of the two-dimensional representations  $\Gamma_*$  or  $\Gamma_{\pm}$  occurs and the associated eigenvalue happens to be real, the anti-unitary symmetry implies a twofold degeneracy

of the energy eigenvalue. Again, the symmetry provides no additional label, and simultaneous eigenstates of  $\hat{H}$  and  $\hat{A}$  can be constructed for  $\Gamma_+$  only. These cases will be denoted by  $\Gamma_*^d$  or  $\Gamma_\pm^d$ .

It will be shown now that the properties of  $\mathcal{PT}$ -symmetric quantum systems are consistent with the representation theory of non-hermitean Hamiltonians possessing an anti-unitary symmetry. Upon identifying

$$\hat{A} = \mathcal{PT}, \quad (23)$$

one needs to check the value of  $(\mathcal{PT})^2$  when applied to eigenstates of the Hamiltonian in order to decide which of the representations  $\Gamma_*$ ,  $\Gamma_\pm$ , or  $\gamma_+$ , is realized. Various explicit examples will be given now.

For parameters  $Z < Z_0^c$ , the eigenvalues of the  $\mathcal{PT}$ -symmetric square-well are real throughout, and the operators  $\hat{H}$  and  $\mathcal{PT}$  have common eigenstates. Thus, the relations (4) correspond to a multiple occurrence of the representation  $\gamma_+$ , compatible with  $(\mathcal{PT})^2 = +\hat{I}$ .

For  $Z > Z_0^c$ , the energy eigenstate  $\psi_0(x) \equiv \langle x|E_0, +\rangle$  in (7) satisfies  $(\mathcal{PT})^2|E_0, +\rangle = +|E_0, +\rangle$ . Therefore, the states  $|E_0, +\rangle$  and  $|E_0, +^*\rangle \equiv \mathcal{PT}|E_0, +\rangle$  carry a representation  $\Gamma_+$ , and the presence of two complex energy eigenvalues,  $E_0$  and  $E_0^*$  is justified. Eqs. (5) can be completed to read:

$$E \neq E^* : \quad \begin{aligned} \hat{H}|E_0, +\rangle &= E_0|E_0, +\rangle, & \mathcal{PT}|E_0, +\rangle &= +|E_0, +^*\rangle, \\ \hat{H}|E_0, +^*\rangle &= E_0^*|E_0, +^*\rangle, & \mathcal{PT}|E_0, +^*\rangle &= +|E_0, +\rangle. \end{aligned} \quad (24)$$

Consequently,  $\mathcal{PT}$ -symmetry is not broken but at  $Z = Z_0^c$  the system switches between the representations  $\Gamma_+$  and  $\gamma_+$ , with a corresponding change of the energy spectrum.

The following examples are taken from a discrete family of non-hermitean operators [7],

$$\hat{H}_M = \hat{p}^2 - (\zeta \cosh 2x - iM)^2, \quad \zeta \in \mathbb{R}, \quad (25)$$

$M$  taking positive integer values. Each operator  $\hat{H}_M$  is invariant under the combined action of  $\mathcal{PT}$  where  $\mathcal{P}$  is parity about the point  $a = i\pi/2$ :  $x \rightarrow i\pi/2 - x$ . Due to the reflection about a point off the real axis, the operators  $\mathcal{P}$  and  $\mathcal{T}$  do not commute as has been pointed out in [8]. However, this fact is not essential here since only the anti-unitary character of the symmetry  $\mathcal{PT}$  is essential.

For  $M = 2$ , two complex conjugate eigenvalues  $E_+$  and  $E_- = E_+^*$  of  $\hat{H}_2$  exist, with associated eigenstates

$$\psi_+(x) = \Psi(x) \cosh x \equiv \langle x|E_+, -\rangle, \quad \psi_-(x) = \Psi(x) \sinh x \equiv \langle x|E_+, -^*\rangle, \quad (26)$$

and a  $\mathcal{PT}$ -invariant function  $\Psi(x) = \exp[(i/2)\zeta \cosh 2x]$ . These states are a flipping pair with flipping value  $i$ ,

$$\mathcal{PT}\psi_+(x) = -i\psi_-(x), \quad \mathcal{PT}\psi_-(x) = i\psi_+(x), \quad (27)$$

and the twofold application of  $\mathcal{PT}$  gives  $(-1)$ . Hence, the representation  $\Gamma_-$  is realized. Similarly, for  $M = 4$ , four eigenstates form two flipping pairs, i.e. two representations  $\Gamma_-$ , each being associated with a pair of complex conjugate eigenvalues.

For  $M = 3$ , three different real eigenvalues of the Hamiltonian  $\hat{H}_3$  have been obtained analytically if  $\zeta^2 < 1/4$ . The corresponding eigenfunctions are given by

$$\psi(x) = \Psi(x) \sinh 2x, \quad \psi_{\pm}(x) = \Psi(x)(A \cosh 2x \pm iB), \quad (28)$$

with real coefficients  $A$  and  $B$ . Under the action of  $\mathcal{PT}$ , the state  $\psi(x)$  is mapped to itself, while  $\psi_{\pm}(x)$  each acquire an additional minus sign. Therefore, the states  $\psi(x) \equiv \langle x|E, +\rangle$  and  $i\psi_{\pm}(x) \equiv \langle x|E_{\pm}\rangle$  are simultaneous eigenstates of  $\hat{H}$  and  $\mathcal{PT}$  with eigenvalues  $+1$ . The part of Hilbert space spanned by these three states transforms according to three copies of the representation  $\gamma_+$ . If  $\zeta = 1/2$ , the eigenvalues  $E_{\pm}$  turn degenerate, and the eigenstates given in (28) merge,  $i\psi_+(x) = i\psi_-(x) \equiv \varphi(x)$ . However, a second, independent  $\mathcal{PT}$ -invariant solution of Schrödinger's equation can be found,

$$\phi(x) = \Psi(x) \int_{x_0}^x dy \frac{e^{-i\varphi(y)/2}}{\varphi^2(y)}. \quad (29)$$

The solutions  $\{\varphi, \phi\}$  transform according to  $\gamma_+ \otimes \gamma_+ \equiv \Gamma_+^d$ . So far, the representation  $\Gamma_*$  has apparently not been realized in  $\mathcal{PT}$ -symmetric quantum systems—a possible explanation is the constraint  $\mathcal{T}^2 = \pm 1$  for time reversal [9].

In summary, the representation theory of anti-unitary symmetries of non-hermitean ‘Hamiltonians’ has been developed on the basis of Wigner’s normal form of anti-unitary operators. Typically, energy eigenvalues come in complex conjugate pairs, and the associated eigenstates of the Hamiltonian span a two-dimensional space carrying one of the two-dimensional representations  $\Gamma_*$ , or  $\Gamma_{\pm}$ . Furthermore, a single real eigenvalue may occur, related to a one-dimensional representation  $\gamma_+$ . In this case a single  $\hat{A}$ -invariant energy eigenstate exists while there are no simultaneous eigenstates of the Hamiltonian and the symmetry operator in the two-dimensional  $\hat{A}$ -invariant subspaces. Instead, flipping pairs of states can be identified. Generally, the symmetry does not imply the existence of degenerate eigenvalues—only if the Hamiltonian happens to have a real eigenvalue, a two-dimensional degenerate subspace may exist occasionally. These results naturally explain the properties of eigenstates and eigenvalues of  $\mathcal{PT}$ -symmetric quantum systems. In particular, it is not necessary to invoke the concept of a *spontaneously broken*  $\mathcal{PT}$ -symmetry. Contrary to a unitary or hermitean symmetry, the presence of an anti-unitary symmetry does not imply the existence of a set of simultaneous eigenstates of  $\hat{H}$  and  $\mathcal{PT}$ —simply because an anti-linear operator is not guaranteed to have a complete set of eigenstates. Finally, the present approach provides a new perspective on the suggested modification of the scalar product in Hilbert space [10] which will be presented elsewhere [11] in detail.

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